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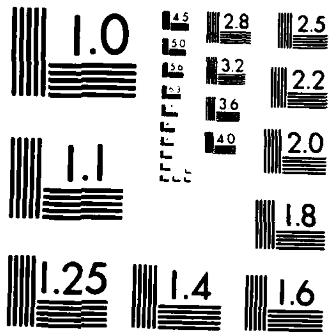

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THE ORIENTATION DISTRIBUTION OF NONSPHERICAL AEROSOL PARTICLES WITHIN A CLOUD

INTERIM REPORT

by Isaiah Gallily

DEPARTMENT OF ATMOSPHERIC SCIENCES
The Hebrew University of Jerusalem
Jerusalem, Israel

November 1984

US Army Armament, Munitions & Chemical Command
Aberdeen Proving Ground, Maryland 21010-5423

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The orientation distribution function of fibrous and platelet-like aerosol particles was calculated for a general laminar flow by solving the Fokker-Plank equation. It has been found that this function shows maxima and minima, which indicates a preferred orientation. The cases of a point source and a laminar jet are brought out as an example.

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PREFACE

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CONTENTS

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THE ORIENTATION DISTRIBUTION OF NONSPHERICAL
AEROSOL PARTICLES WITHIN A CLOUD

1. GENERAL

The orientation distribuiton function F of nonspherical aerosol particles is very decisive for many cloud properties such as light scattering and radiative transfer (1,2), diffusional transport mechanics (3-5) and average rate of sedimentation (6).

It is also very important in rheology for the constitutive properties of non-Newtonian fluids (7-9).

In general, the orientation function is affected by two opposing physical factors: The randomizing action of the rotational Brownian motion (or micro-turbulent eddies) and the orienting influence of flow gradient.

Up to now, the studied situations were those of the (asymptotic) weak and strong field in which the rotational Peclet number α which indicates the ratio between the above factors, viz. $\alpha = W^{\circ} / D^{*}$ was

$\alpha \ll 1$ or $\alpha \gg 1$. Likewise,

the investigations were rather concerned with the simple shear flows.

2. AIM OF STUDY

Since many cases of significance are characterized by values of α of the order of unity, as occurs in the free atmosphere and with typically-sized particles, it became of interest to study these cases. In addition, the general laminar field where the nine components of the gradient tensor had to be treated once for its own significance and second time for employing it in models for the real, turbulent atmosphere.

3. BASIC EQUATIONS AND ASSUMPTIONS

The basic equation in the reported study was the (source-free) Fokker-Planck equation of conservation in angle-space

$$\partial F / \partial t + \nabla \cdot (F \boldsymbol{\omega} - \mathbf{D} \cdot \nabla F) = 0 \quad . \tag{1}$$

*For nomenclature see Appendix

We have considered a system of small spheroidal particles immersed in a general laminar flow which is given in their vicinity by the linear relationship.

$$\mathbf{u}(\mathbf{x},t) = \mathbf{W}(t) \cdot \mathbf{x} \quad . \tag{2}$$

The small particles simulate (asymptotically) straight long fibers or flat platelets which are used in many applications.
The rotational velocity of the particles $\boldsymbol{\omega}$ of Eq.[1] was taken to be given by the Jeffery's equation (10)

$$\omega_i = \frac{1}{2}\left[V'_{kj} + S'_{kj}\,(a_j^2 - a_k^2)/(a_j^2 + a_k^2)\right] \tag{3}$$

where $i, j, k \rightarrow 1,2,3$ are cyclic permutation indices, a_i, a_j, a_k are the semi-axes of the ellipsoids, $V'_{ij} = W'_{ij} - W'_{ji}$; $S'_{ij} = W'_{ij} + W'_{ji}$; $W'_{ij} = \partial u'_i / \partial x'_j$ and $\mathbf{u}'(\mathbf{x},t)$, $\mathbf{x}$ are respectively the (fluid) velocities and location vector in the body-locked coordinate system $\mathbf{x}'$ (Fig.1)

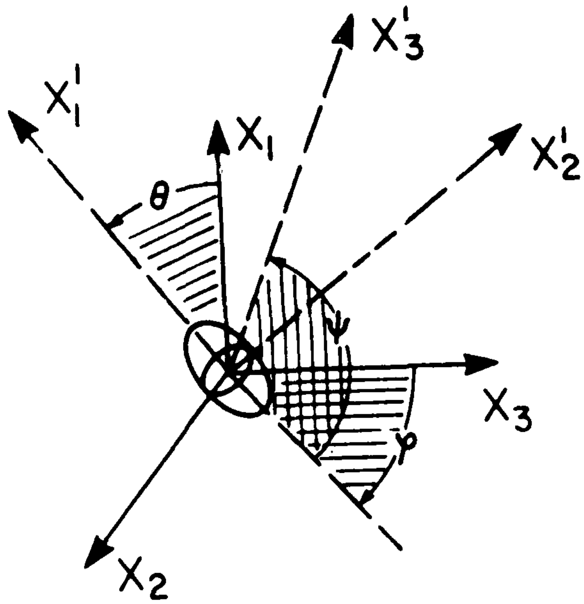

Fig. 1. The two coordinate systems, $\mathbf{x}'$ (body locked) and $\mathbf{x}$ (external) used in the analysis; φ, θ, ψ -Eulers' angles

Here, using the usual kinematic relationships between θ, φ ($\Psi = 0$) and ω_1', ω_2', ω', and the similarity transformation between the x' and x systems, we finally obtained that

$$\dot{\varphi} = V/2 + ctg\,(E_{31}\,c\varphi - E_{21}\,s\varphi) - \lambda\,(S_{32}\,c_2\varphi - Q_1\,s_2\varphi)$$

and

$$\dot{\theta} = G_{2131}\,c^2\theta - G_{1213}\,s^2\theta + \frac{\lambda}{2}\,s_2\theta\,(Q_2 + Q_1\,c_2\varphi + S_{32}\,s_2\varphi) \tag{4}$$

in which $E_{ik} = \frac{1}{2}(V_{ik} + \lambda S_{ik})$, $G_{ijkl} = E_{ij}\,c\varphi + E_{kl}\,s\varphi$,

$Q_1 = \frac{1}{2}(W_{22} - W_{33})$, $Q_2 = \frac{1}{2}(W_{22} + W_{33} - 2W_{11})$, $V_{ik} = W_{ik} - W_{ki}$,

$S_{ik} = W_{ik} - W_{ki}$, $W_{ik} = \partial u_i/\partial x_k$, $c_m\varphi = \cos m\varphi$, $c^m\varphi = \cos^m\varphi$,

$s_m\varphi = \sin m\varphi$, $s^m\varphi = \sin^m\varphi$ etc., $\lambda = (R^2 - 1)/(R^2 + 1)$, $R = a_1/a_2$.

Now, after non-dimensionalization by designating $\tilde{W}_{ik} = W_{ik}/W_0$ and $\tilde{t} = t\,W_0$ (W_0 - a typical gradient component), we could convert the Fokker-Planck equation to the form*

*The $\sim$ sign is dropped out for the sake of simplicity.

$$\partial F/\partial t + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(F\dot{\theta}\sin\theta) + \frac{\partial}{\partial\varphi}(F\dot{\varphi}) = \Delta F/\alpha \qquad (5)$$

where D is the mid-diameter rotational diffusion coefficient of the axially symmetric particles. The normalization condition was taken, as ususal, to be

$$\int_0^{2\pi}\int_0^{\pi} F\sin\theta\, d\theta\, d\varphi = 1 \quad . \qquad (6)$$

4. SOLUTION OF THE FOKKER-PLANCK EQUATION

According to the theory of Fourier series, we wrote down the solution to Eq. [5] as a series of spherical harmonics

$$F = \sum_{n=0}^{\infty}\sum_{m=0}^{n}(1-\tfrac{1}{2}\delta_{m0})\left[A_{0n}^{m}(t)\,c\ \varphi + A_{1n}^{m}(t)\,s\ \varphi\right]\ P_n^m(c\theta) \quad . \qquad (7)$$

Thus, inserting [7] into [5] and taking account of the symmetry properties of the physical problem, we obtained for the A-coefficients the set of the simultaneous equations

$$\frac{dA_{kn}^{m}}{dt} = -\frac{n(n+1)}{\alpha}A_{kn}^{m} - \sum_{j=n-2}^{n+2}\sum_{p=m-2}^{m+2}\sum_{\ell=1}^{2}(1+\delta_{m0})$$

$$\times\left[D_{\ell,jn}^{pm}\ A_{kj}^{m} + (-1)^{k}C_{\ell,jn}^{pm}\ A_{1-k,j}^{p}\right] \qquad (8)$$

in which $D_{\ell,jn}^{pm}$, $C_{\ell,jn}^{pm}$ are functions of S_{ik} , V_{ik} , Q_1, Q_2 and the size parameter λ defined above.*

The latter were numerically solved by the employment of a fast differential equations-solver based on an extrapolation method of Burlish and Stoer.(11) It turned out that our general solution included previous work as special cases.

*See Proceedings of the 1983 CSL Scientific Conference, Aberdeen Proving Ground, MD (to be published).

5. NUMERICAL RESULTS

Considering realistic situations of particles with a characteristic size of $r \sim 10^{-5} - 10^{-3}$ cm. (whose computed D is $D \sim 1 \ \mathrm{sec}^{-1}$), typical flow velocities and gradients of 1-10 $\mathrm{m.sec}^{-1}$ and 1-10 sec^{-1}, respectively, we came out with Peclét number values of $\alpha \sim$ 1-10.

As indicative examples, we bring out here the cases of:

i. A point source flow whose velocity is given by

$$\mathbf{u} = q_0 \mathbf{r} / 4\pi r^3 \tag{9}$$

and whose gradient is

$$W = \frac{\delta_{ik}}{r^3} - \frac{3 x_i x_j}{r^5} \tag{10}$$

where x_i is normalized by a typical length r_0, $\mathbf{r}(x_i)$ is the radius vector, $W_0 = q_0 / 4\pi r_0^3$ and q_0 a constant.

ii. A round laminar jet whose axial (u_1) and radial (u_r) velocity components are (12)

$$u_1 = \frac{2 \gamma^2 \nu}{x_1} f(\xi) \tag{11}$$

and

$$u_r = \frac{\gamma \nu \xi}{x_1} (1 - \xi^2/4) f(\xi) \tag{12}$$

and the gradient components are

$$W_{11} = -\eta\,(1 - 3\xi^2/4), \quad W_{1r} = -\gamma\,\eta\,\xi \ , \quad W_r = W_{11}\,\xi/\gamma ,$$

$$W_{rr} = \frac{1}{2}\,\eta\left(1 - \frac{3}{2}\xi^2 + \frac{\xi^4}{16}\right) + \frac{u_r}{r} \qquad (13)$$

where $\xi = \gamma r / x_1$, $f(\xi) = (1 + \xi^2/4)^{-2}$, γ is determined by the jets' momentum J , $J = (16/3)\,\pi\,\rho\,\gamma^{-2}\,\nu^2$, r is the radial distance (again) and r , x_i are later on non-dimensionalized by r_0 .

Indicative results for these two significant flows are presented in Figs. 2,3 and 4,5 in which a preferred orientation of the considered particles is clearly seen by the pronounced maxima of F.

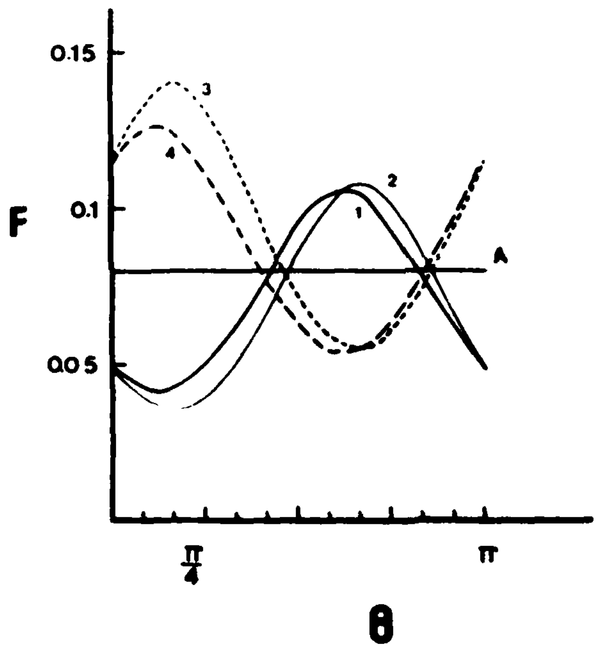

Fig. 2. The orientation distribution function F vs the (Euler) angle θ in a point source flow $\alpha = 1$, $R = 0.02$ (platelets) and R = 50 (straight fibers).

$\tilde{t}\ (= t\,W_0) \geq 2$, $x_1 = 1$, $x_2 = x_3 = 0.4$; A - t = 0 (random orientation);

——, $R = 50$: 1 - $\varphi = 0$, 2 - $\varphi = \pi/4$; — —, $R = 0.02$: 3 - $\varphi = 0$, 4 - $\varphi = \pi/4$.

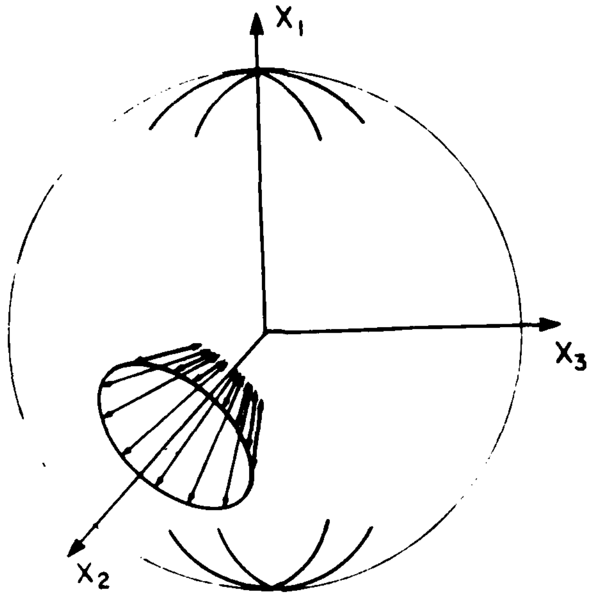

Fig 3. A perspective view of particle orientation in a point source field (schematical)

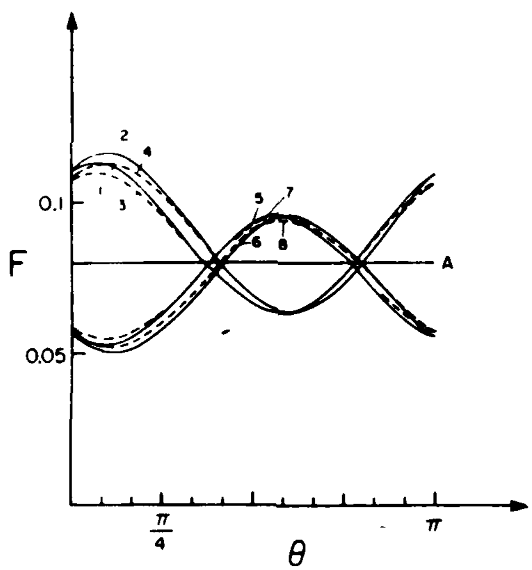

Fig. 4. The orientation distribution function F vs the(Euler) angle θ in a flow of a laminar, axi-symmetric jet $\alpha = 1$, $R = 0.01, 0.2, 5, 100$.

$\tilde{t} = (t W_0) \geq 2$, $x_1 = 1$, $x_2 = x_3$, $\xi = 0.5$, $\gamma = 1$, $\varphi = 0, \pi/4$.

$1 - R = 0.01, \varphi = 0$; $2 - R = 0.01, \varphi = \pi/4$; $3 - R = 0.2, \varphi = 0$;

$4 - R = 0.2, \varphi = \pi/4$; $5 - R = 5, \varphi = 0$; $6 - R = 5, \varphi = \pi/4$;

$7 - R = 100, \varphi = 0$; $8 - R = 100, \varphi = \pi/4$.

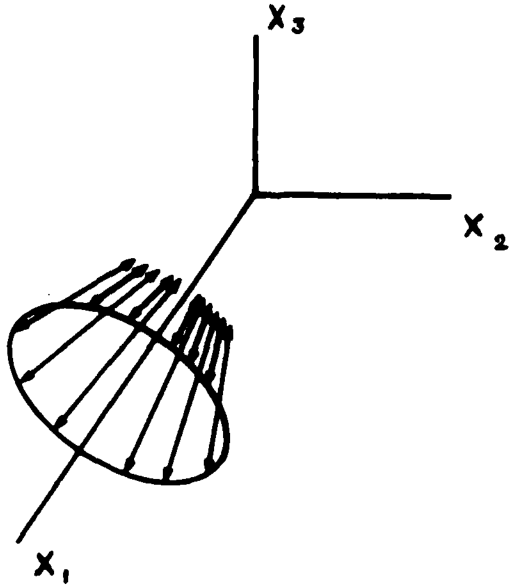

Fig. 5. A perspective view of particle orientation in a laminar jet (schematical)

6. SUMMARY

The orientation distribution function of fibrous and platelet-like aerosol particles was calculated for a general laminar flow by solving the Fokker-Planck equation.

It has been found that this function shows maxima and minima, which indicates a preferred orientation. The cases of a point source and a laminar jet are brought out as an example.

7. FUTURE PLANS

Based on the reported study, the next stage of research on the orientation within a turbulent cloud is now in progress.

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APPENDIX. NOMENCLATURE

a_i, a_j, a_k - half axes of an ellipsoidal particle

A^m_{on}, A^m_{1n} - coefficients in expansion as spherical harmonics

$C^{pm}_{\ell,jn}$ $D^{pm}_{\ell,jn}$ - coefficients in Eq. [8]

$\mathbf{D}$, D - rotational diffusion tensor and coefficient, respectively

$E_{ik}, G_{ijk\ell}, a_1, a_2$ - defined in text

F - orientation distribuiton function

i, j, k, ℓ, m, p - indices

$\mathbf{r}$ -radius vector; r_o - normalizing radius vector

$R = a_1/a_2$

S'_{ik}, S_{ik} - defined in text

t - time

$\mathbf{u}$ - flow velocity

V'_{ik}, V_{ik} - defined in text

W'_{ik}, W_{ik} - component of the gradient tensor; -normalizing component

$\mathbf{x}'$, $\mathbf{x}$ - location vectors.

Greek Letters

α – rotational Peclet numbers

γ – parameter related to jet's momentum

δ_{ij} – Kroneckers' delta

φ, θ, ψ – Eulers' angles

$\boldsymbol{\omega}$ – rotational velocity of the particle

∇ – nabla operator in angle-space

Δ – Laplacian operator in angle-space

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